

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -12.6 °C

Global applicability domain: Inside

Local applicability domain index: 9.86e-01

Confidence level: 9.25e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dodecane</div> <div>Measured: -9.60</div> <div>Predicted: -12.6</div>	<div>Image not found</div> <div>Tridecane</div> <div>Measured: -5.30</div> <div>Predicted: -4.65</div>	<div>Image not found</div> <div>Undecane</div> <div>Measured: -25.6</div> <div>Predicted: -14.0</div>
<div>Image not found</div> <div>Tetradecane</div> <div>Measured: 5.80</div> <div>Predicted: 3.94</div>	<div>Image not found</div> <div>Decane</div> <div>Measured: -29.7</div> <div>Predicted: -25.8</div>	